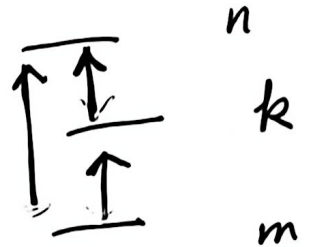


Lecture 2: Heisenberg's magic

§1: Reinterpretation of kinematic variable

$$X_{n,m} e^{i\omega(n,m)t}$$

$$= \begin{pmatrix} x_{11} e^{i\omega_{11}t} & x_{12} e^{i\omega_{12}t} & \dots \\ x_{21} e^{i\omega_{21}t} & x_{22} e^{i\omega_{22}t} & \dots \\ \vdots & \vdots & \ddots \end{pmatrix}$$



$$(X^2)_{nm} = \sum_k (X)_{nk} (X)_{km}$$

$$\omega_{nm} = \omega_{nk} + \omega_{km}$$

Ritz combination law

$$\ddot{x} + f(x) = 0 \leftarrow \text{in the matrix sense}$$

§ Quantization

$$\frac{1}{2\pi} \oint p dq = n\hbar$$

$\longleftrightarrow$

$$\frac{\hbar}{2m} = \sum_{\alpha=0}^{\infty} \{ \omega(n+\alpha, n) |X(n+\alpha, n)|^2 - \omega(n, n-\alpha) |X(n, n-\alpha)|^2 \}$$

§ Heisenberg's zero point motion $[(\dot{x})^2]_{nn} = \frac{\hbar\omega}{m} (n+1/2)$

§ Born - Jordan's matrix mechanics

$$[x, p] = i\hbar \leftarrow \text{Born's tomb stone}$$

Heisenberg's breakthrough

①

① Interpret electron coordinate x as the relation between initial and final states

← light emission

consider transition $n \rightarrow n-l$ ($l > 0$), x is represented

$$X_{n-l,n}(t) = X_{n-l,n} e^{-i\omega_{n-l \leftarrow n} t}$$

according to EM, electron oscillation frequency is the light frequency. Consider the classic expansion

$$X_n(t) = \sum_l X_n(l) e^{-il\omega_n t}$$

We can make a correspondence

$$\boxed{\begin{array}{l} X_{n-l,n} e^{-i\omega_{n-l \leftarrow n} t} \\ \leftrightarrow X_n(l) e^{-il\omega_n t} \end{array}}$$

For $l=0$, $X_{n,n}$ corresponds to the zero frequency part of $X_n(t)$.

hence $X_{n,n}$ should be real.

Consider the light absorption, i.e. $l < 0$

$$\boxed{X_{n,n-|l|} e^{-i\omega_{n \leftarrow n-|l|} t} \leftrightarrow X_n(-|l|) e^{i|l|\omega_n t}}$$

Note $\omega_{n \leftarrow n-l} = -\omega_{n-l \leftarrow n}$, but not $\omega_{n+l \leftarrow n} = -\omega_{n-l \leftarrow n}$

↑
typically not true

Classical relation: $X_n(-l) = X_n^*(l)$

Correspondingly, $X_{n,n-l} = X_{n-l,n}^*$, or $\boxed{X_{nm} = X_{mn}^*}$

②

$$X_{mn}(t) e^{-i\omega_{m \leftarrow n} t} \leftrightarrow \begin{pmatrix} X_{11} & X_{12} e^{-i\omega_{1 \leftarrow 2} t} & \dots \\ X_{21} e^{-i\omega_{2 \leftarrow 1} t} & X_{22} & \dots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

Reinterpretation of kinematic coordinate

② Reconstruct the relation x^2 and x

$$\begin{aligned} (X^2)_{mn} e^{-i\omega_{m \leftarrow n} t} &= \sum_k X_{m,k} e^{-i\omega_{m \leftarrow k} t} X_{k,n} e^{-i\omega_{k \leftarrow n} t} \\ &= \sum_k X_{mk} X_{kn} e^{-i\omega_{m \leftarrow n} t} \quad \leftarrow \text{Ritz combination} \\ &\quad \uparrow \\ &\quad \text{matrix product} \end{aligned}$$

Reinvention of matrix! $x \rightarrow x^2 \rightarrow x^n$

③ reinterpretation of equation of motion

Heisenberg thought the Hamilton Eq should be valid.
We should maintain the form of dynamic Eq, but use the matrix interpretation

$$\ddot{X}_{mn} + [f(x)]_{mn} = 0$$

For the harmonic oscillator, $\ddot{X}_{mn} + \omega_0^2 X_{mn} = 0.$

③

④ reinterpretation of Bohr quantization

$$\oint p dx = nh \Rightarrow m \oint \dot{x}^2 dt = nh$$

$$X_n(t) = \sum_{\ell=-\infty}^{\infty} X_n(\ell) e^{-i\ell\omega_n t} \rightarrow \dot{X}_n(t) = \sum_{\ell} (-i\ell\omega_n) X_n(\ell) e^{-i\ell\omega_n t}$$

$$\dot{x}^2 = \sum_{\ell} \ell^2 \omega_n^2 |X_n(\ell)|^2 + \sum_{\ell \neq \ell'} \ell \ell' \omega_n^2 X_n(\ell) X_n^*(\ell') e^{-i(\ell-\ell')\omega_n t}$$

$$m \oint \dot{x}^2 dt = m \sum_{\ell} \ell^2 \omega_n^2 |X_n(\ell)|^2 \oint dt \leftarrow T = \frac{2\pi}{\omega_n}$$

$$= \boxed{2\pi m \sum_{\ell} \ell^2 \omega_n |X_n(\ell)|^2 = nh}$$

Consider the limit $n \rightarrow \infty$, and the harmonic order $|\ell| \ll n$.

We view 'n' as continuous, and take derivative

$$\frac{\hbar}{m} = \frac{d}{dn} \sum_{\ell} \ell^2 \omega_n |X_n(\ell)|^2 = \sum_{\ell} \ell \frac{d}{dn} [\ell \omega_n |X_n(\ell)|^2]$$

Since $\ell \ll n$, $\ell \frac{d}{dn} \rightarrow$ difference

$$\ell \frac{d}{dn} [\ell \omega_n |X_n(\ell)|^2] = \ell \omega_{n+\ell} |X_{n+\ell}(\ell)|^2 - \ell \omega_n |X_n(\ell)|^2$$

$$\Rightarrow \frac{\hbar}{m} = \sum_{\ell=-\infty}^{\infty} [\omega_{n \leftarrow n+\ell} |X_{n, n+\ell}|^2 - \omega_{n-\ell \leftarrow n} |X_{n-\ell, n}|^2]$$

$$\omega_{n \leftarrow n+\ell} = -\omega_{n, n-\ell}, \quad |X_{n-\ell, n}|^2 = |X_{n, n-\ell}|^2$$

and $\omega_{n \leftarrow n} = 0$

$$\begin{aligned} \ell < 0 \text{ part: } & \omega_{n \leftarrow n-|\ell|} |X_{n, n-|\ell|}|^2 - \omega_{n+|\ell| \leftarrow n} |X_{n+|\ell|, n}|^2 \\ & = \omega_{n \leftarrow n+|\ell|} |X_{n+|\ell|, n}|^2 - \omega_{n-|\ell| \leftarrow n} |X_{n, n-|\ell|}|^2 \end{aligned}$$

(4)

We combine and simplify $\Rightarrow$

$$\frac{\hbar}{2m} = \sum_{l=0}^{\infty} (\omega_{n \leftarrow n+l} |X_{n+l,n}|^2 - \omega_{n-l \leftarrow n} |X_{n,n-l}|^2)$$

f - sum rule, which is equivalent to $[X, p] = i\hbar$ later by Born and Jordan.

(*) Application — harmonic oscillator

$$\ddot{x}_{n+l,n}(t) + \omega_0^2 x_{n+l,n}(t) = 0 \Rightarrow x_{n+l,n}(t) = x_{n+l,n} e^{-i\omega_{n+l \leftarrow n} t}$$

$$\Rightarrow (\omega_0^2 - \omega_{n \leftarrow n \pm l}^2) X_{n,n \pm l} = 0$$

For non-vanishing matrix elements, we should

$$\text{have } \omega_{n \leftarrow n \pm l} = \pm \omega_0.$$

For 1d motion, energy increases with action, i.e. there is at most one "l", such that $X_{n,n \pm l} \neq 0$. If there exist two, $\omega_0 = \omega_{n \leftarrow n+l} = \omega_{n \leftarrow n+l'}$, then $l' = l$.

In the limit $n \rightarrow +\infty$, according to the correspondence principle

$$\omega_{n \leftarrow n \pm 1} = \pm \omega_0, \Rightarrow X_{n,n \pm 1} \text{ can be nonzero.}$$

For harmonic oscillator, frequency is independent on amplitude

$$\partial E / \partial J = \omega_0, \text{ hence, } \omega_{n \leftarrow n \pm 1} = \pm \omega_0 \text{ should be maintained}$$

even at n is small.

(5)

Then the f-sum rule:

$$\frac{\hbar}{2m} = \omega_0 [|X_{n+1,n}|^2 - |X_{n,n-1}|^2]$$

$$\frac{\hbar}{2m} = \omega_0 [|X_{n,n-1}|^2 - |X_{n-1,n-2}|^2]$$

$$\vdots$$

$$\frac{\hbar}{2m} = \omega_0 [|X_{1,0}|^2]$$

since all the $|X_{n+1,n}|^2$ are positive, this sequence must be bound from below. we denote $n \geq 0$.

$$\Rightarrow |X_{1,0}|^2 = \frac{\hbar}{2m\omega_0}, \quad |X_{n+1,n}|^2 = \frac{\hbar}{2m\omega_0} (n+1)$$

For the moment, we assume that $X_{n+1,n}$ is real

$$\Rightarrow \begin{cases} X_{n+1,n} = \sqrt{\frac{\hbar}{2m\omega_0}} (n+1) \\ X_{n-1,n} = \sqrt{\frac{\hbar}{2m\omega_0}} n \end{cases} \quad (n \geq 1)$$

$$\begin{aligned} X_{n+1,n}(t) &= X_{n+1,n} e^{i\omega_0 t} \\ X_{n-1,n}(t) &= X_{n-1,n} e^{-i\omega_0 t} \end{aligned}$$

(*) Zero point motion

$$\oint p dq = m \int_0^T (\dot{x})^2 dt$$

$$(\dot{x}^2)_{nn} = \sum \dot{X}_{nm} \dot{X}_{mn} = \dot{X}_{n,n-1} \dot{X}_{n-1,n} + \dot{X}_{n,n+1} \dot{X}_{n+1,n}$$

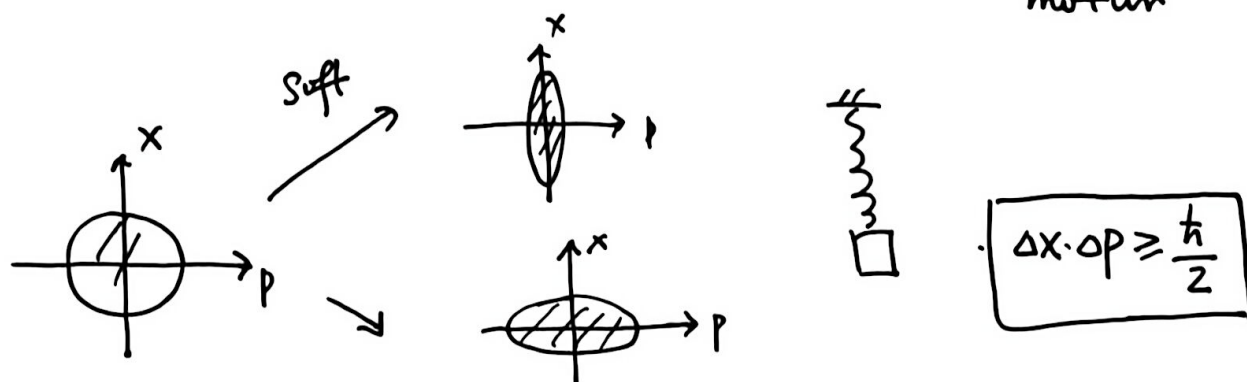
$$X_{n,n-1} = \left(\frac{n\hbar}{2m\omega_0} \right)^{1/2} e^{i\omega_0 t} \Rightarrow \dot{X}_{n,n-1} = i\omega_0 \left(\frac{n\hbar}{2m\omega_0} \right)^{1/2} e^{i\omega_0 t}$$

$$(\dot{x}^2)_{nn} = \omega_0^2 \left[\frac{n\hbar}{2m\omega_0} + \frac{(n+1)\hbar}{2m\omega_0} \right] = \frac{\hbar\omega_0}{m} (n+1/2)$$

$$J = \left(\oint p dq \right)_{nn} = \hbar\omega_0 (n+1/2) \int_0^T dt = 2\pi\hbar (n+1/2) = (n+1/2) h$$

(6)

Since $\omega = \frac{\partial E}{\partial J} \Rightarrow \boxed{E = (n + 1/2) \hbar \omega}$ $\leftarrow \frac{1}{2} : \text{zero point motion}$



(*) Born-Jordan commutation

x, p do not commute: if they are matrices, $xp - px = m(\dot{x}\dot{x} - \dot{x}x)$

check diagonal part $(x\dot{x} - \dot{x}x)_{nn}$,

$$\sum_l x_{n,n-l} \dot{x}_{n-l,n} - \dot{x}_{n,n-l} x_{n-l,n}$$

$$= \sum_l |x_{n,n-l}|^2 (-i\omega_{n-l \leftarrow n}) - (-i\omega_{n \leftarrow n-l}) |x_{n-l,n}|^2$$

if $l > 0, \sum_{l>0} -2i\omega_{n-l \leftarrow n} |x_{n,n-l}|^2$

if $l < 0, \sum_{|l|>0} |x_{n,n+|l|}|^2 (-2i\omega_{n+|l| \leftarrow n})$

$$\Rightarrow (x\dot{x} - \dot{x}x)_{nn} = +2i \sum_{l>0} [\omega_{n+l \leftarrow n} |x_{n+l,n}|^2 - \omega_{n-l \leftarrow n} |x_{n,n-l}|^2]$$

$$= \frac{\hbar}{m} i$$

$$\Rightarrow \boxed{(xp - px)_{nn} = i\hbar}$$